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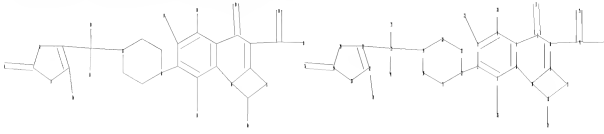


chain nodes :
13 14 15 16 23 24 25 26 27 33 34 35 36
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 17 18 19 20 21 22 28 29 30 31 32
chain bonds :
1-26 2-22 3-23 4-24 7-13 8-14 12-25 14-15 14-16 19-27 27-33 27-34 27-31 29-36 32-35
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 9-11 10-12 11-12 17-18 17-22 18-19 19-20 20-21 21-22 28-29 28-32 29-30 30-31 31-32
exact/norm bonds :
2-22 5-7 6-10 7-8 7-13 8-9 9-10 9-11 10-12 11-12 14-15 14-16 17-18 17-22 18-19 19-20 19-27 20-21 21-22 28-29 28-32 29-30 29-36 30-31 31-32
exact bonds :
1-26 3-23 4-24 8-14 12-25 27-33 27-34 27-31 32-35
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:CLASS 34:CLASS 35:CLASS 36:CLASS

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 13:21:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 13:22:55 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 23 TO ITERATE

100.0% PROCESSED 23 ITERATIONS 12 ANSWERS
SEARCH TIME: 00.00.01

L3 12 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 184.34 184.55

FILE 'CAPLUS' ENTERED AT 13:24:26 ON 27 MAY 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 27 May 2008 VOL 148 ISS 22
FILE LAST UPDATED: 26 May 2008 (20080526/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l3
L4 192 L3

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 1.44 185.99

FILE 'REGISTRY' ENTERED AT 13:25:57 ON 27 MAY 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 MAY 2008 HIGHEST RN 1022798-85-1
DICTIONARY FILE UPDATES: 26 MAY 2008 HIGHEST RN 1022798-85-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

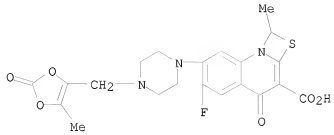
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> s l3 and ref.caplus>10
427861 REF.CAPLUS>10
L5 1 L3 AND REF.CAPLUS>10

=> d l5

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 123447-62-1 REGISTRY
ED Entered STN: 27 Oct 1989
CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,3-Dioxole, 1H,4H-[1,3]thiazeto[3,2-a]quinoline-3-carboxylic acid deriv.
OTHER NAMES:
CN (±)-7-[4-[(Z)-2,3-Dihydroxy-2-butenyl]-1-piperazinyl]-6-fluoro-1-methyl-4-oxo-1H,4H-[1,3]thiazeto[3,2-a]quinoline-3-carboxylic acid, cyclic carbonate
CN NM 441
CN Prulifloxacin
CN Quisnon
CN Sword
MF C21 H20 F N3 O6 S
CI COM
SR CA
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CBNB, CHEMCATS, CIN, DDFU, DRUGU, EMBASE, IMSDRUGNEWS, IMSPATENTS, IMSPRODUCT, IMSRESEARCH, IPA, MEDLINE, MRCK*, PHAR, PROMT, PROUSDDR, PS, RTECS*, SCISEARCH, SYNTHLINE, TOXCENTER, USAN, USPATFULL
(*File contains numerically searchable property data)
Other Sources: WHO



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

192 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
192 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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=> s l3 not l5
L6          11 L3 NOT L5

=> s l6 and acetonitrile
        135826 ACETONITRILE
L7           1 L6 AND ACETONITRILE

=> d l7

L7   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   791105-27-6  REGISTRY
ED   Entered STN:  01 Dec 2004
CN   1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid,
     6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-
     piperazinyl]-4-oxo-, acetonitrile (1:1)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid,
     6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-
     piperazinyl]-4-oxo-, compd. with acetonitrile (1:1) (9CI)
MF   C21 H20 F N3 O6 S . C2 H3 N
SR   CA
LC   STN Files:   CA, CAPLUS, USPATFULL

     CM   1

     CRN  123447-62-1
     CMF  C21 H20 F N3 O6 S
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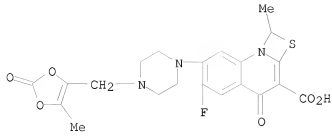

CM 2

CRN 75-05-8
CMF C2 H3 N

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	10.53	196.52

FILE 'CAPLUS' ENTERED AT 13:27:56 ON 27 MAY 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 27 May 2008 VOL 148 ISS 22
FILE LAST UPDATED: 26 May 2008 (20080526/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l7
L8 1 L7

=> d l8 bib abs

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:965259 CAPLUS
DN 141:415959
TI Preparation of crystals of quinolinecarboxylic acid derivative solvate
IN Akai, Jun; Nishida, Hiroshi
PA Nippon Shinyaku Co. Ltd., Japan
SO PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004096815	A1	20041111	WO 2004-JP6216	20040428
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004234287	A1	20041111	AU 2004-234287	20040428
	CA 2523854	A1	20041111	CA 2004-2523854	20040428
	EP 1626051	A1	20060215	EP 2004-730102	20040428
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	BR 2004009930	A	20060425	BR 2004-9930	20040428
	CN 1780842	A	20060531	CN 2004-80011455	20040428
	IN 2005CN02801	A	20070525	IN 2005-CN2801	20051031
	US 20070149540	A1	20070628	US 2006-555039	20060912
PRAI	JP 2003-124643	A	20030430		
	JP 2004-6057	A	20040113		
	WO 2004-JP6216	W	20040428		

AB This invention provides crystals of 6-fluoro-1-methyl-7-[4-(5-methyl-2-oxo-1,3-dioxolen-4-yl)methyl-1-piperazinyl]-4-oxo-4H-[1,3]thiazeto[3,2-a]quinoline-3-carboxylic acid acetonitrile solvate (compound B) which is useful as an intermediate for producing preferentially III-type crystals of 6-fluoro-1-methyl-7-[4-(5-methyl-2-oxo-1,3-dioxolen-4-yl)methyl-1-piperazinyl]-4-oxo-4H-[1,3]-thiazeto[3,2-a]quinoline-3-carboxylic acid (compound A). Crystals of compound B show diffraction peaks at 7.3°, 14.7°, 19.2°, 22.3°, etc. Compound B can be preferentially crystallized from acetonitrile by controlling the supersatn. concentration, and desolvation of the crystals of compound B can give III-type crystals of compound A. Compound A is a known antibacterial agent.

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s l6 not l7
7 L6

```
             1 L7
L9           6 L6 NOT L7

=> s l9 and acetonitrile/ab,bi
         50566 ACETONITRILE/AB
         95129 ACETONITRILE/BI
L10          0 L9 AND ACETONITRILE/AB,BI

=> d l9 1-6 bib abs hitstr

L9   ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   2001:472467  CAPLUS
DN   135:71252
TI   Use of chemotherapeutic agents for the topical and/or local treatment of
     diseases caused by bacteria
IN   Schulz, Hans-Herrmann; Schlimbach, Gunther
PA   Germany
SO   PCT Int. Appl., 59 pp.
     CODEN: PIXXD2
DT   Patent
LA   German
FAN.CNT 1
     PATENT NO.          KIND   DATE       APPLICATION NO.         DATE
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PI   WO 2001045679       A2     20010628   WO 2000-EP13155         20001222
     WO 2001045679       A3     20020718
          W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
              CR, CU, CZ, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
              ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
              LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,
              SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,
              ZA, ZW
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
              DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
              BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     DE 19962470         A1     20010712   DE 1999-19962470        19991222
     CA 2395459          A1     20010628   CA 2000-2395459         20001222
     EP 1244434          A2     20021002   EP 2000-985241          20001222
     EP 1244434          B1     20040317
          R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2000017041       A      20021022   BR 2000-17041           20001222
     JP 2004501063       T      20040115   JP 2001-546418          20001222
     EP 1408034          A1     20040414   EP 2003-28047           20001222
     EP 1408034          B1     20070808
          R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, FI, CY, TR
     AT 261722           T      20040415   AT 2000-985241          20001222
     PT 1244434          T      20040831   PT 2000-985241          20001222
     ES 2218264          T3     20041116   ES 2000-985241          20001222
     CN 1668598          A      20050914   CN 2000-819067          20001222
     AU 784496           B2     20060413   AU 2001-21716           20001222
     AT 369344           T      20070815   AT 2003-28047           20001222
     ES 2291583          T3     20080301   ES 2003-28047           20001222
     NO 2002003026       A      20020820   NO 2002-3026            20020621
     NO 323727           B1     20070702
     MX 2002PA06248      A      20021205   MX 2002-PA6248          20020621
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	US 20030045544	A1	20030306	US 2002-168441	20020621
	ZA 2002005027	A	20040308	ZA 2002-5027	20020621
	KR 803442	B1	20080213	KR 2002-708087	20020621
	IN 2002MN00856	A	20050304	IN 2002-MN856	20020624
	AU 2005202737	A1	20050721	AU 2005-202737	20050623
	US 20070197501	A1	20070823	US 2007-619823	20070104
	NO 2007001958	A	20020820	NO 2007-1958	20070417
PRAI	DE 1999-19962470	A	19991222		
	AU 2001-21716	A3	20001222		
	EP 2000-985241	A3	20001222		
	WO 2000-EP13155	W	20001222		
	US 2002-168441	A3	20020621		

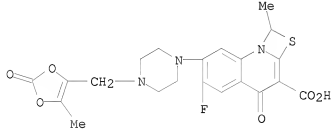
OS MARPAT 135:71252

AB The invention relates to the use of chemotherapeutic agents for the production of a medicament for the topical and/or local treatment or prophylaxis of diseases caused by bacteria in humans or animals.

IT 123447-63-2 123447-64-3 346586-42-3
346586-84-3 346587-07-3 346587-35-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(chemotherapeutic agents for topical and/or local treatment of diseases caused by bacteria)

RN 123447-63-2 CAPLUS

CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 123447-64-3 CAPLUS

CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, monomethanesulfonate (9CI) (CA INDEX NAME)

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CRN 123447-62-1
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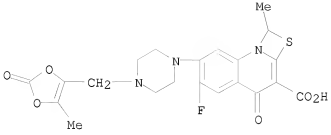
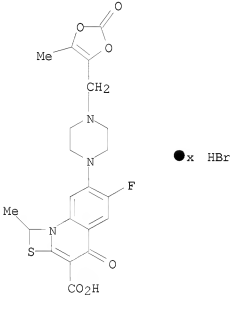


CM 2

CRN 75-75-2
CMF C H4 O3 S

RN 346586-42-3 CAPLUS
CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, hydrobromide (9CI) (CA INDEX NAME)



RN 346586-84-3 CAPLUS
CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid,

6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

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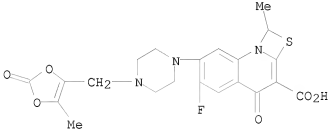
CRN 123447-62-1
CMF C21 H20 F N3 O6 S



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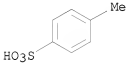
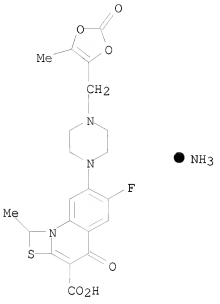
CRN 104-15-4
CMF C7 H8 O3 S



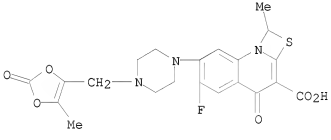
RN 346587-07-3 CAPLUS
CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, ammonium salt (9CI) (CA INDEX NAME)



RN 346587-35-7 CAPLUS
CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, compd. with guanidine (1:1) (CA INDEX NAME)

CM 1

CRN 123447-62-1
CMF C21 H20 F N3 O6 S

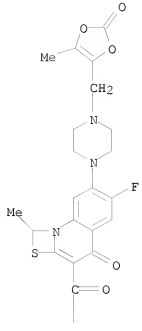


CM 2

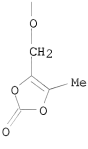
CRN 113-00-8
CMF C H5 N3

L9 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1997:104301 CAPLUS
DN 126:203641
TI Chemical structure, physicochemical properties and stability of prulifloxacin
AU Kakemi, Kazuo; Aoki, Naoko; Mikawa, Miyako; Iizuka, Yasushi; Kiyama, Yasunori; Okamoto, Takashi; Hamakawa, Tomoaki; Shimidzu, Naoki
CS Research Laboratories, Nippon Shinyaku Co., Ltd., Kyoto, 601, Japan
SO Iyakuhin Kenkyu (1997), 28(1), 1-11
CODEN: IYKEDH; ISSN: 0287-0894
PB Nippon Koteisho Kyokai
DT Journal
LA Japanese
AB A new antibacterial agent, prulifloxacin, was studied to clarify its chemical structure and physicochem. properties. The physicochem. properties were clarified by studying its solubility in various solvents, hygroscopicity, powder x-ray diffraction pattern, polymorphism, pKa, partition coeffs. and thermal anal. An HPLC method for the assay of prulifloxacin and anal. of related compds. was established. In the solid state, prulifloxacin was stable to heat. However, it was slightly unstable to moisture and light. In solns. of various pH values at 40°, prulifloxacin decomposed to NM394.
IT 173599-92-3, NM 603
RL: ANT (Analyte); ANST (Analytical study)
(structure and physicochem. properties and stability of prulifloxacin)
RN 173599-92-3 CAPLUS
CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl ester (CA INDEX NAME)

PAGE 1-A

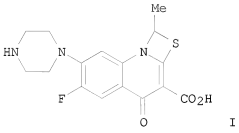


PAGE 2-A



L9 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1995:966987 CAPLUS
DN 124:175087
OREF 124:32462h,32463a
TI Studies on synthesis of the antibacterial agent NM441 . II. Selection of a suitable base for alkylation of 1-substituted piperazine with 4-(bromomethyl)-5-methyl-1,3-dioxol-2-one
AU Fujii, Tatsuya; Nishida, Hiroshi; Abiru, Yoshiaki; Yamamoto, Masashi; Kise, Masahiro
CS Res. Lab., Nippon Shinyaku Co., Ltd., Kyoto, 601, Japan
SO Chemical & Pharmaceutical Bulletin (1995), 43(11), 1872-7
CODEN: CPBTAL; ISSN: 0009-2363
PB Pharmaceutical Society of Japan

DT Journal
LA English
GI



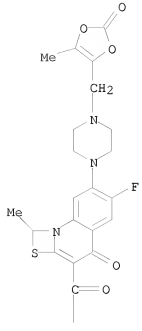
AB Diisopropylamine (DIPA), N,N-diisopropylethylamine (DIPEA), tributylamine (TNBA) and 7-(1-piperazinyl)-4-quinolone-3-carboxylic acid (I) were titrated in water-dimethylformamide (DMF) mixts. containing 45-98% DMF. Apparent pKa values in anhydrous DMF (pKDMF) were calculated by extrapolation from the variation in the half-neutralization pH values in aqueous DMF. The validity of the relative basicity derived from the pKDMFs was confirmed by examination of the kinetics of esterification of a derivative of I with 4-(bromomethyl)-5-methyl-1,3-dioxol-2-one (DMDO-Br). Relative basicities in DMF were: the carboxylate anion of I >> DIPA > DIPEA > TNBA > the amino group in the piperazinyl part of I. This order is clearly different from that observed in water. It is concluded that DIPEA is a suitable agent to suppress the undesired esterification during the reaction to mask the amino group of I with a DMDO group, because it does not remove a proton from the carboxyl group, but only from the protonated amino group.

IT 173599-92-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(esterification of antibacterial agent NM441 with 4-(bromomethyl)-5-methyl-1,3-dioxol-2-one)

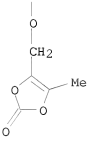
RN 173599-92-3 CAPLUS

CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L9 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1994:507691 CAPLUS
DN 121:107691
OREF 121:19423a,19426a
TI Studies on synthesis of antibacterial agent (NM441). I. Kinetics and mechanism of the reaction of 4-(bromomethyl)-5-methyl-1,3-dioxol-2-one with 1-substituted piperazine (NM394)
AU Nishida, Hiroshi; Fujii, Tatsuya; Abiru, Yoshiaki; Yatsuki, Katsuya; Yamamoto, Masashi; Shimizu, Naoki; Kakemi, Kazuo; Mikawa, Miyako; Kise, Masahiro
CS Res. Lab., Nippon Shinyaku Co., Ltd., Kyoto, 601, Japan
SO Bulletin of the Chemical Society of Japan (1994), 67(5), 1419-26
CODEN: BCSJA8; ISSN: 0009-2673

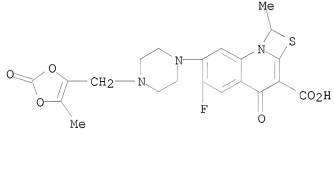
DT Journal
LA English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB When a tertiary amine (I) is synthesized from 4-bromomethyl-5-methyl-1,3-dioxol-2-one (DMDO-Br) and a secondary amine (II) in DMF, the quaternary ammonium salt III, the ring-opened compound IV, and the 1,2-adduct V are formed as byproducts. I is formed by nucleophilic attack of II on the carbon α to the bromine atom of DMDO-Br. The ring-opened compound IV is formed by nucleophilic attack of II on the carbonyl carbon of DMDO-Br. The quaternary ammonium salt III is formed by the reaction of DMDO-Br with I (the Menshutkin reaction). Main pathway for the formation of V is the Michael addition of II to IV. Kinetics of the reactions have been studied and the methods to obtain I suppressing the formations of III-V have been proposed based on the kinetic results.

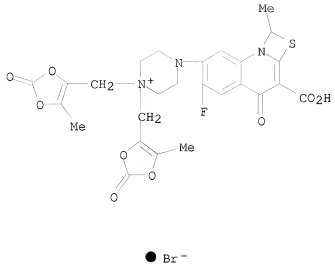
IT 123447-63-2P 156834-56-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 123447-63-2 CAPLUS
CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

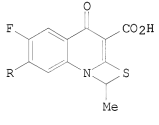


● HCl

RN 156834-56-9 CAPLUS
CN Piperazinium, 4-(3-carboxy-6-fluoro-1-methyl-4-oxo-1H,4H-[1,3]thiazeto[3,2-a]quinolin-7-yl)-1,1-bis[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-, bromide (9CI) (CA INDEX NAME)



L9 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1993:6894 CAPLUS
DN 118:6894
OREF 118:1465a,1468a
TI Studies on pyridonecarboxylic acids. 1. Synthesis and antibacterial evaluation of 7-substituted-6-halo-4-oxo-4H-[1,3]thiazeto[3,2-a]quinoline-3-carboxylic acids
AU Segawa, Jun; Kitano, Masahiko; Kazuno, Kenji; Matsuoka, Masato; Shirahase, Ichiro; Ozaki, Masakuni; Matsuda, Masato; Tomii, Yoshifumi; Kise, Masahiro
CS Res. Lab., Nippon Shinyak Co., Ltd., Kyoto, 601, Japan
SO Journal of Medicinal Chemistry (1992), 35(25), 4727-38
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 118:6894
GI



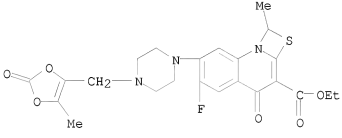
AB A series of [1,3]thiazeto[3,2-a]quinoline-3-carboxylic acids (I) and their esters were prepared and evaluated for antibacterial activity. The derivs. with an H or Me group at C-1, F at C-6, and a piperazinyl or 4-methyl-1-piperazinyl group at C-7 showed superior in vitro antibacterial activity, and the derivs. with 4-methyl-1-piperazinyl group at C-7 had

potent in vivo activity. I (R = piperazino) (NM394) showed excellent in vitro antibacterial activity and low toxicity but poor absorption from the gastrointestinal tract. I [R = (5-methyl-2-oxo-1,3-dioxol-4-yl)methylpiperazino) (NM441) had a favorable pharmacokinetic profile and oral activity superior to that of ciprofloxacin in exptl. animals.

IT 123447-61-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)

RN 123447-61-0 CAPLUS

CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, ethyl ester (CA INDEX NAME)



L9 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1989:594791 CAPLUS

DN 111:194791

OREF 111:32387a,32390a

TI Preparation and testing of 6-fluoro-7-piperazino-4-oxo-4H-[1,3]thiazeto[3,2-a]quinolinecarboxylate derivatives as antibactericides

IN Kise, Masahiro; Kitano, Masahiko; Ozaki, Masakuni; Kazuno, Kenji; Matsuda, Masahito; Shirahase, Ichiro; Segawa, Jun

PA Nippon Shinyaku Co., Ltd., Japan

SO Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 315828	A1	19890517	EP 1988-117810	19881026
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JP 01294680	A	19891128	JP 1988-263568	19881019
JP 07051579	B	19950605		
AT 74608	T	19920415	AT 1988-117810	19881026
ES 2031569	T3	19921216	ES 1988-117810	19881026
ZA 8808186	A	19890726	ZA 1988-8186	19881101
AU 8824673	A	19890511	AU 1988-24673	19881103
AU 608911	B2	19910418		
DK 8806163	A	19890508	DK 1988-6163	19881104
DK 172077	B1	19971013		
CN 1033055	A	19890524	CN 1988-107689	19881105

	CN 1024194	B	19940413		
	FI 8805128	A	19890508	FI 1988-5128	19881107
	FI 88618	B	19930226		
	FI 88618	C	19930610		
	NO 8804958	A	19890508	NO 1988-4958	19881107
	NO 177934	B	19950911		
	NO 177934	C	19951220		
	CA 1316925	C	19930427	CA 1988-582460	19881107
	IL 88303	A	19930513	IL 1988-88303	19881107
	US 5086049	A	19920204	US 1991-682434	19910408
PRAI	JP 1987-281550	A	19871107		
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OS CASREACT 111:194791; MARPAT 111:194791

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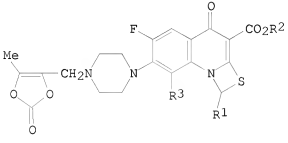


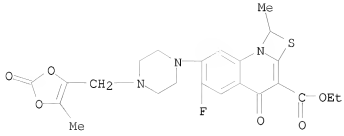
I

AB The title compds. [I; R1 = H, alkyl, (substituted) Ph; R2 = H, alkyl; R3 = H, halo, alkoxy], useful as antibacterials, were prepared Et 6-fluoro-1-methyl-4-oxo-7-piperazino-4H-[1,3]thiazeto[3,2-a]quinolinecarboxylate and KHCO3 in DMF were treated with 4-bromomethyl-5-methyl-1,3-dioxolen-2-one with ice cooling. The mixture was stirred 3 h to give I (R1 = Me, R2 = Et, R3 = H). I had oral ED50's in mice of 0.0152-0.427 mg against P. aeruginosa, vs. 0.692 for ofloxacin.

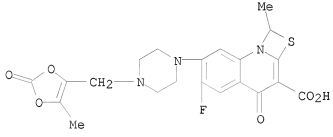
IT 123447-61-0P 123447-63-2P 123447-64-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antibacterial)

RN 123447-61-0 CAPLUS

CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, ethyl ester (CA INDEX NAME)



RN 123447-63-2 CAPLUS
CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 123447-64-3 CAPLUS
CN 1H,4H-[1,3]Thiazeto[3,2-a]quinoline-3-carboxylic acid, 6-fluoro-1-methyl-7-[4-[(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl]-1-piperazinyl]-4-oxo-, monomethanesulfonate (9CI) (CA INDEX NAME)

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CRN 123447-62-1
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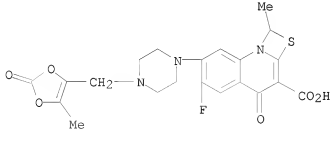

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L6          11 S L3 NOT L5
L7           1 S L6 AND ACETONITRILE

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        32201 SOLVATE?/BI
L11          0 L9 AND SOLVATE?/AB,BI

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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)
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  This file contains CAS Registry Numbers for easy and accurate
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  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

  New CAS Information Use Policies, enter HELP USAGETERMS for details.

  This file supports REGistRY for direct browsing and searching of
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  more information.

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     (FILE 'HOME' ENTERED AT 13:15:47 ON 27 MAY 2008)

     FILE 'REGISTRY' ENTERED AT 13:16:07 ON 27 MAY 2008
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L2           0 S L1
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     FILE 'CAPLUS' ENTERED AT 13:24:26 ON 27 MAY 2008
L4         192 S L3

     FILE 'REGISTRY' ENTERED AT 13:25:57 ON 27 MAY 2008
L5           1 S L3 AND REF.CAPLUS>10
L6          11 S L3 NOT L5
L7           1 S L6 AND ACETONITRILE

     FILE 'CAPLUS' ENTERED AT 13:27:56 ON 27 MAY 2008
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CA SUBSCRIBER PRICE                                    0.00      -5.60

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FILE COVERS 1907 - 27 May 2008 VOL 148 ISS 22
FILE LAST UPDATED: 26 May 2008 (20080526/ED)

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L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:965259 CAPLUS
DN 141:415959
TI Preparation of crystals of quinolinecarboxylic acid derivative solvate
IN Akai, Jun; Nishida, Hiroshi
PA Nippon Shinyaku Co. Ltd., Japan
SO PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004096815	A1	20041111	WO 2004-JP6216	20040428
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     EP 1626051             A1    20060215    EP 2004-730102          20040428
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     US 20070149540         A1    20070628    US 2006-555039          20060912
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     JP 2004-6057           A     20040113
     WO 2004-JP6216         W     20040428
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              ALL CITATIONS AVAILABLE IN THE RE FORMAT


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CA SUBSCRIBER PRICE                                     0.00      -5.60

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